Tight-binding calculation for the AlAs–GaAs (100) interface

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We report the results of a study of the electronic properties of the AlAs–GaAs interface using the tight-binding method. The tight-binding matrix for the superlattice system is used in the limit in which the thickness of the repeated superlattice slab becomes large. This system is studied in detail with special emphasis placed on the determination of interface states. No interface states with energies within the GaAs forbidden gap are found. The densities of states per layer are calculated and compared with bulk densities of states. They resemble the bulk densities of states except for layers adjacent to the interface.

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I. INTRODUCTION

Interfaces and superlattices have been the subject of much recent experimental and theoretical study.[1–5] Much of the experimental work has been carried out on the AlAs/GaAs system. In some ways this system provides an ideal system for theoretical study since the structure is probably as close to being an abrupt interface with the atoms in their bulk crystal positions as for any physical system.[6] Hence, the very difficult yet important question of spatial arrangement of atoms at the interface is in large part circumvented.

In this paper we report on a study of the electronic properties of the interface formed parallel to (100) crystal planes using the tight-binding method. The calculation is done for a superlattice system of alternating slabs of AlAs and GaAs in the limit in which the slab thicknesses become large. Interface states (states having non-zero amplitudes only on atomic layers near the interface) are clearly secn for the superlattice consisting of ten atomic layers of AlAs alternating with ten of GaAs. No interface states are found with energies within the forbidden gap of bulk GaAs. A layer density of states calculation for each layer of the superlattice shows that the densities of states are bulklike except for those layers right adjacent to the interface.

II. TIGHT-BINDING CALCULATION

The tight-binding calculation used a limited basis set of four localized orbitals per atom, one orbital of s-type symmetry and three of p-type symmetry (P_x,P_y,P_z) for each anion (As) and cation (Al,Ga). Four valence bands and four conduction bands (each doubly degenerate) are thus calculated. Explicit forms for the orbitals were not used. Instead, the Hamiltonian matrix elements were parameterized assuming the above wave function symmetries. These parameters were determined separately for AlAs and GaAs by fitting the resulting energies to bulk pseudopotential calculations.[7,8] A good fit to the valence-band structure was obtained from these parameters. The conduction bands were more difficult to duplicate. The parameters were chosen to reproduce the correct band gaps in the bulk materials. The shapes of the conduction bands, however, only roughly resembled their pseudopotential counterparts. Our parameter fitting procedure did not uniquely determine the parameters chosen. As a check on our results several sets of parameters were used for the same calculation. The results we report did not vary qualitatively with the different sets of parameters. Energy values varied slightly, but the same features were found with the different sets. The precise values of the parameters used for the results presented here are given in Ref. 2. One more parameter, the relative energy positions of the valence band maxima in the two semiconductors, was needed. This parameter takes into account the average potential difference between the two. Its effect is to determine the heights of the energy barriers formed by the larger band-gapped AlAs to electrons and holes at the band-gap edges of GaAs. Dingle, Gossard, and Weig-

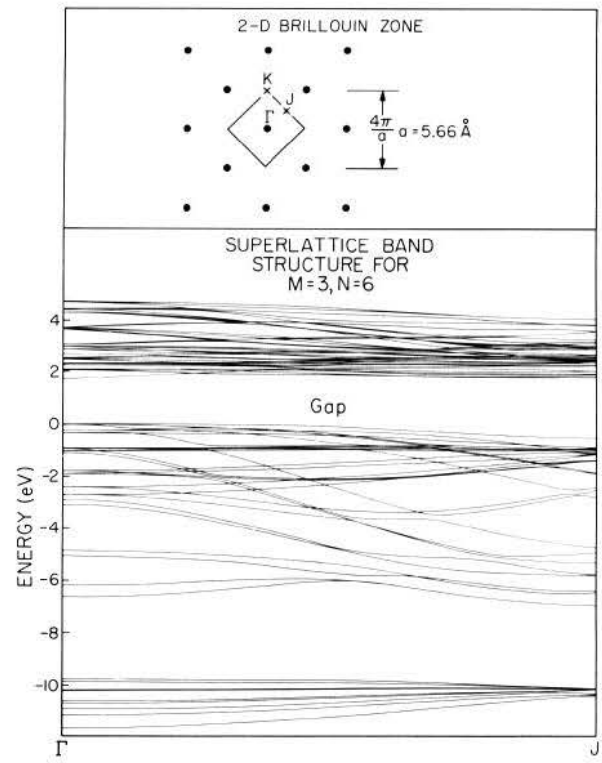

FIG. 1. Band structure of AlAs–GaAs superlattice consisting of three layers of AlAs alternating with six monolayers of GaAs from Γ to J. The inset shows a two-dimensional slice of the Brillouin zone parallel to the interface. a = 5.66 Å.

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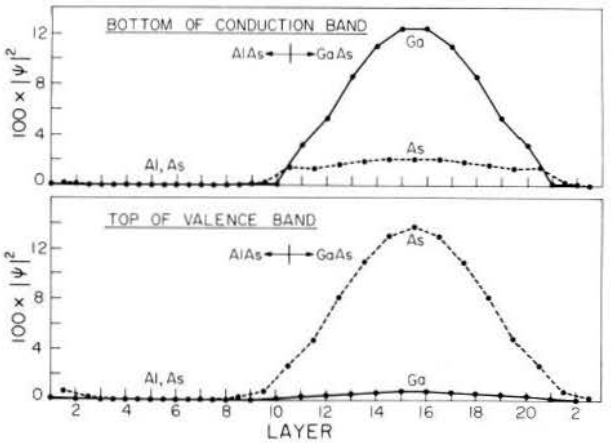

FIG. 2. Charge distributions for the two band edge states for the $M = N = 10$ superlattice with separate curves for Al, Ga, and As.

mann[9] have found that the valence-band offset is approximately 15% of the band-gap difference for GaAs–$Ga_{1-x}Al_xAs$ for x between 0.19 and 0.27. We have extrapolated their results to AlAs/GaAs and assumed that the offset is 15% of the difference between our calculated band gaps. It was assumed that there was no displacement of the atoms from the bulk positions at the interface.

III. RESULTS

Figure 1 shows the band structure for the superlattice consisting of three layers of AlAs alternating with six layers of GaAs ($M = 3$, $N = 6$). The inset shows the two-dimensional slice of the Brillouin zone parallel to the interface and including the $\mathbf{k} = 0$ point. The energy bands are shown from Γ to J as indicated. The number of bands is $M + N$ times the number of bulk bands, because the superlattice unit cell is $M + N$ times as large as the bulk cell. Other directions including the direction perpendicular to the interface are as easily calculated. The dispersion of the bands in this direction is considerably less, however, because the width of the Brillouin zone is $M + N$ times less than in the other two directions. Some of the electronic wave functions for this superlattice are substantially localized at the interfaces. The slabs are too thin, however, to definitely categorize them as interface states.

The charge densities for the states at the top of the valence band and the bottom of the conduction band for the $M = N = 10$ superlattice are shown in Fig. 2. Separate densities are plotted for Al, Ga, and As. These states are similar to the corresponding states in bulk GaAs in that they have similar s and p character and anion to cation ratios. The well-like character of the potential at the band edges results in the peaked character of the states in the GaAs slabs. There are also states with nearby energies having a double-peaked structure, representing the next higher well states.

Interface states in the valence band were found at and near the Brillouin zone edges. By interface states we mean states which die away within two or three atomic layers from the interface layers. The J point was found to be particularly rich in interface states. These states had energies which were split off from energy bands associated with the bulk band structures as shown in Fig. 3. Fig. 3(c) shows the valence-band structure for the $M = N = 10$ superlattice from three quarters of the way from Γ to J. In Figs. 3(a) and (b) are shown the corresponding band structures of AlAs–AlAs and GaAs–GaAs superlattices. Figure 3(c) is seen to be a superposition of Figs. 3(a) and (b) with four split-off bands indicated by arrows. The two higher energy interface states are associated with the two high concentrations of bands at the zone edge lying between them. All the interface states share the same symmetries as the bands from which they are split off, and are thus identifiable as being associated with them. The interface states are located below the valence band edge which is indicated in Fig. 3(c). Interface states were also found near the zone edges in other directions in k-space. In all cases these states had a localized nature only near the zone edges. No interface states were found at or near the Γ-point.

The densities of states for bulk AlAs and GaAs and the layer densities of states for the $M = N = 7$ superlattice are shown in Fig. 4. Layers 1–7 are the AlAs slab and layers 8–14 the GaAs slab. Layers 4 and 11 are in the middle of the AlAs and GaAs slabs, respectively, and are similar to the bulk densities of states for those materials. Layers 7 and 14 are interface layers and their densities of states have contributions from both AlAs and GaAs as well as the interface states. Layers

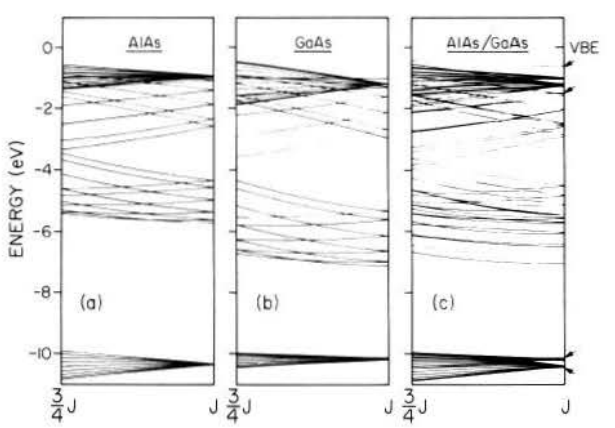

FIG. 3. Valence band structure near the J point for $M = N = 10$ superlattices consisting of (a) all AlAs, (b) all GaAs, (c) AlAs–GaAs.

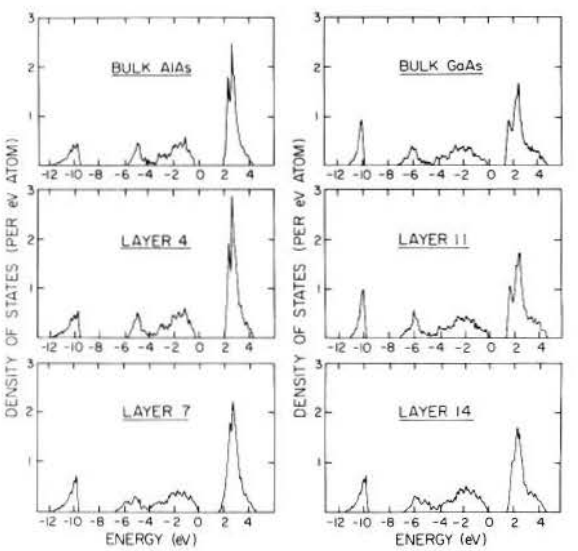

FIG. 4. Densities of states for bulk AlAs and bulk GaAs and layer densities of states for the $M = N = 7$ superlattice.

adjacent to these interface layers are clearly identifiable as being either AlAs- or GaAs-like in character. Interface states make a contribution to the layer densities of states near the interface, but are not identifiable as separate peaks. The layer densities of states in each slab approximately resemble the corresponding bulk densities of states for AlAs and GaAs.

IV. CONCLUSIONS

We found no evidence for the existence of interface states within the forbidden gap of GaAs. Interface states in the valence bands were found, but with energies which might make them difficult to detect experimentally. Modification of the electronic structure from bulklike as shown in the layer densities of states occurs only in the layers at the interface.

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